

Exact Curie temperature for the Ising model on Archimedean and Laves lattices

Alessandro Codello

August 30, 2010

Institut für Physik, Johannes Gutenberg-Universität, Mainz

Abstract

Using the Feynman-Vdovichenko combinatorial approach to the two dimensional Ising model, we determine the exact Curie temperature for all two dimensional Archimedean lattices. By means of duality, we extend our results to cover all two dimensional Laves lattices. For those lattices where the exact critical temperatures are not exactly known yet, we compare them with Monte Carlo simulations.

1 Introduction

As a solvable example of a statistical system exhibiting a second order phase transition, the Ising model has been of central importance in the development of statistical mechanics and still continues to play a key role as test ground for new theoretical and computational methods.

The existence of a Curie point, at which a transition from the paramagnetic phase to the ferromagnetic phase takes place, as the temperature is lowered, was first proven to exist by Peierls [1] in the case of the square lattice Ising model. Successively Kramers and Wannier [2] calculated the value of the critical temperature using duality and the property of the square lattice of being self-dual. With the first calculation of the zero field free energy by Onsager [3, 4] and the calculation of the spontaneous magnetization by Yang

[5], the second order character of the phase transition was established. This successful attempt to solve the Ising model on a square lattice was carried over using transfer matrix techniques. Along the same path, Wannier was first to study the triangular and hexagonal (also called honeycomb) lattice Ising model, in particular in relation to antiferromagnetism studies [6]. The first non regular lattice zero field free energy was calculated for the “Kagome” lattice by Kano and Naya [7]. Successively the “extended Kagome” lattice was studied by Soyzi [8]. The “Union Jack” lattice and the dual, the “Bathroom-tile” lattice, were covered by [9, 10]. Other lattices were investigated in [11, 12].

A combinatorial approach to solve the Ising model was proposed by Kac and Ward [14]. It is based on the possibility to map the high temperature expansion of the partition function onto a particular random-walk problem on the lattice. Feynman [15] and Vodvichenko [16] showed how to recover the Onsager solution by this method. The above mapping is based on a topological theorem about loops on two dimensional lattices proven by Sherman [17].

Despite of many efforts, the free energy in presence of a non-zero external magnetic field has not yet been calculated exactly. Some results are available only at criticality $T = T_c$ or for weak magnetic field $B \rightarrow 0$ [23]. Still nowadays the Ising model is an active area of research.

In this prospect any exact analytical result can be useful. In this paper we use the combinatorial method to calculate the Curie temperatures for the Ising model on all Archimedean lattices and all their duals, the Laves lattices. This method was first used by Thompson and Wardrop [19] to calculate the critical temperatures for two Archimedean lattices, here we calculate the Curie temperature for all of them, including three values which were known by now only approximately from Monte Carlo simulations.

2 Archimedean and Laves lattices

Archimedean lattices are uniform tilings of the plane in which all the faces are regular polygons and the symmetry group acts transitively on the vertices. It follows that all vertices are equivalent and have the same coordination number z . Also, all vertices are shared by the same set of polygons and thus we can associate to each Archimedean lattice a set of integers (p_1, p_2, \dots) indicating, in cyclic order, the polygons meeting at a given vertex [20]. When a polygon appears more than one time consecutively, for example as in (\dots, p, p, \dots) , we abbreviate the notation writing (\dots, p^2, \dots) . In this way, the uniform tilings of the plane, made with squares, triangles and hexagons, are indicated respectively by (4^4) , (3^6) and (6^3) .

It is possible to show, that apart the regular tilings just listed, there are eight other

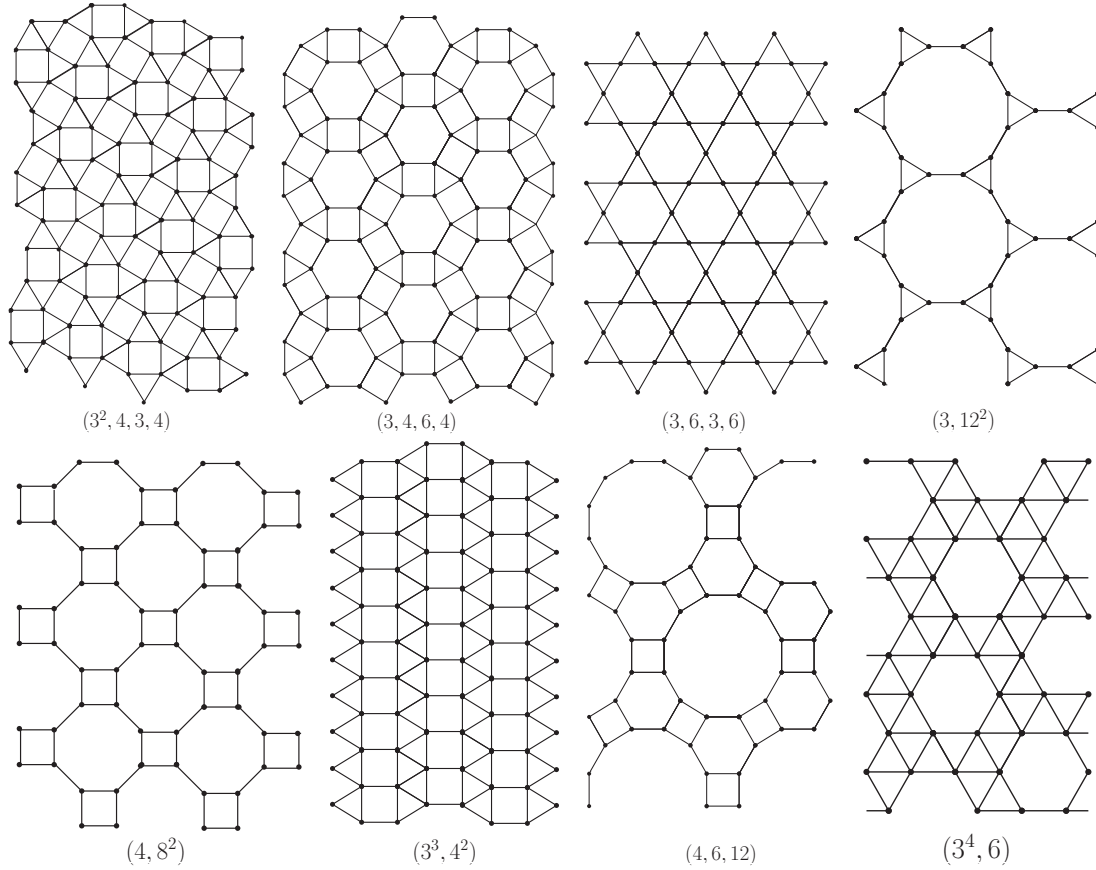


Figure 1: The eight uniform tilings of the plane made with more than one regular polygon.

uniform tilings of the plane. These are all constructed using more than one regular polygon and are shown in Figure 1. In total we have eleven different two dimensional Archimedean lattices. Some of these lattices have names: “Kagome” $(3, 6, 3, 6)$, “extended Kagome” $(3, 12^2)$ and “Bathroom-tile” $(4, 8^2)$, while the others have no particular name. Note that the lattice $(3^4, 6)$ is the only non-specular one.

The dual lattice Λ^* of a given lattice Λ is constructed associating a vertex of Λ^* to each face of Λ . The duals of the Archimedean lattices are called Laves lattices. They are tilings of the plane made with one non-regular polygon and are indicated by the notation $[p_1, p_2, \dots]$. The square lattice is self-dual $[4^4] = (4^4)$ (this property was used by Kramers and Wannier to first calculate the critical temperature for this lattice), while the triangular and hexagonal lattices are dual of each other $[3^6] = (6^3)$, $[6^3] = (3^6)$. Of the duals of the other uniform lattices, three are triangular tilings, two are rhomboidal tilings and three are pentagonal tilings. The dual of the Kagome lattice $[3, 6, 3, 6]$ is called “Dice lattice” and the lattice $[4, 8^2]$, dual to the “Bathroom tile” lattice, is called “Union Jack” lattice.

3 Ising model

We briefly review the definition of the model and the basic steps involved in the combinatorial solution of it. At every lattice site i a spin variable $\sigma_i \in \{-1, 1\}$ is located and a microstate is defined by a spin configuration $\{\sigma\}$. Nearest neighbor interactions are assumed so that the energy of a given spin configuration is given by

$$E\{\sigma\} = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j - B \sum_i \sigma_i. \quad (1)$$

If $J > 0$ the interaction is ferromagnetic, while it is antiferromagnetic if $J < 0$. For the aim of calculating the Curie temperature, we can set to zero the external applied magnetic field $B = 0$. The partition function is the sum over all spin configurations, weighted by the Boltzman-Gibbs factor

$$Z_\Lambda = \sum_{\{\sigma\}} \exp \left\{ K \sum_{\langle i,j \rangle} \sigma_i \sigma_j \right\}. \quad (2)$$

We defined $K = J/k_B T$ where k_B is the Boltzmann constant.

Using the high temperature expansion, the partition function (2), can be rewritten as:

$$Z_\Lambda = 2^N (\cosh K)^{N_E} \Phi_\Lambda(v). \quad (3)$$

In (3) we defined $v = \tanh K$, while N is the number of lattice sites and $N_E = \frac{z}{2}N$ is the number of links per lattice site. The function $\Phi_\Lambda(v)$ is the generating function of the numbers G_n (we define $G_0 = 1$), which count the graphs of length n with even vertices that can be drawn on the lattice Λ . In this way, the problem of solving the Ising model on Λ is reduced to the combinatorial problem of counting even closed graphs on Λ .

If we don't care about the fact that we have to count only over closed graphs with even vertices, we can use the standard combinatorial property that the sum over all (possibly disconnected) closed graphs, is given by the exponential of the sum over only connected closed graphs. But connected closed graphs can be seen as closed random-walk paths. If we find a way to consider in the sum only closed paths with even vertices, we have a way to calculate the generating function $\Phi_\Lambda(v)$ simply by counting closed random-walks paths.

Feynman [15] and Vodvicenko [16] introduced a trick to count only over paths with even vertices: weight the random-walk with a complex amplitude $\alpha = e^{i\theta/2}$ at every turn of angle θ the random-walker makes along his trajectory. In this way all contributions coming from non-even paths delete each other in the sum, and the mapping from the high temperature expansion to the random-walk problem works out correctly (see [25, 24]

Λ	z	p	m
$(3, 12^2)$	3	6	18
$(4, 6, 12)$	3	12	36
$(4, 8^2)$	3	4	12
(6^3)	3	2	6
$(3, 4, 6, 4)$	4	6	24
(4^4)	4	1	4
$(3, 6, 3, 6)$	4	3	12
$(3^4, 6)$	5	6	30
$(3^3, 4^2)$	5	2	10
$(3^2, 4, 3, 4)$	5	4	20
(3^6)	6	1	6

Table 1: Coordination number z , number of lattice sites per unit cell p and size m of the random-walk matrix \mathbf{W}_Λ for each Archimedean lattice.

for more details). This results have a rigorous base on a topological theorem proven by Sherman [17] and were further investigated by Morita [18].

After introducing the appropriate amplitudes, which depend on the properties of the lattice Λ , we need to count all connected closed graphs of length n that can be draw on Λ . This number is equal to the number of random-walks of length n starting from all the lattice sites

$$\frac{1}{2n} \sum_{\mathbf{x}_0, i_0} N_{i_0}(\mathbf{x}_0, \mathbf{x}_0, n), \quad (4)$$

where $N_i(\mathbf{x}, \mathbf{x}_0, n)$ is the number of walks arriving at site \mathbf{x} from direction i at the n -th step starting from site \mathbf{x}_0 . The sum is over all possible starting points and the factor $\frac{1}{2n}$ exclude the over-counting due to the fact that there are two directions in which a graph can be travelled and the fact that each graph can be seen as a random-walk starting from all of the sites of the lattice reached by the random-walker.

The random-walk problem can be written in terms of the master equation

$$N_i(\mathbf{x}, \mathbf{x}_0, n) = \sum_{\mathbf{x}', j} W_{i,j}(\mathbf{x}, \mathbf{x}') N_j(\mathbf{x}', \mathbf{x}_0, n-1), \quad (5)$$

with boundary conditions $N_i(\mathbf{x}, \mathbf{x}_0, 0) = \delta_{\mathbf{x}, \mathbf{x}_0} \delta_{i, i_0}$. Equation (5) is solved by $N_i(\mathbf{x}, \mathbf{x}_0, n) = W_{i, i_0}^n(\mathbf{x}, \mathbf{x}_0)$. From equation (4) we find, in the limit $N \rightarrow \infty$, the explicit form for the generating function:

$$\Phi_\Lambda(v) = \exp \left\{ \frac{N}{2} \int \frac{d^2 k}{(2\pi)^2} \log \det [\mathbf{1} - v \mathbf{W}_\Lambda(k_x, k_y)] \right\},$$

where the integration is over the region $0 \leq k_x \leq 2\pi$ and $0 \leq k_y \leq 2\pi$. The free energy

z	Λ	$P_\Lambda(v)$
3	$(3, 12^2)$	$(1+v)^4(1-2v+3v^2-2v^3-2v^4)^2$
	$(4, 6, 12)$	$(1+2v^2+5v^4)^2(1-2v^2+2v^4-10v^6+v^8)^2$
	$(4, 8^2)$	$(1-v-v^2)(1+v+2v^2)(1-4v^3-v^4)$
	(6^3)	$(1-3v^2)^2$
4	$(3, 4, 6, 4)$	$(1-v^2)^2(1+v^2)^6(1-4v^2-6v^4-4v^6+v^8)$
	$(3, 6, 3, 6)$	$(1-v^2)^2(1-4v^2-6v^4-4v^6+v^8)$
	(4^4)	$(1-2v-v^2)^2$
5	$(3^4, 6)$	$(1+v)^8(1+3v^2)^2(1-4v+7v^2-12v^3+3v^4-3v^6)^2$
	$(3^3, 4^2)$	$(1+v)^2(1-3v)^2(1+v^2)^2$
	$(3^2, 4, 3, 4)$	$(1+v)^4(1-2v-v^2-4v^3-9v^4+6v^5-7v^6)^2$
6	(3^6)	$(1+v)^2(1-4v+v^2)^2$

Table 2: The polynomials $P_\Lambda(v)$ as defined in equation (7), for each Archimedean lattice.

for spin $f_\Lambda = F_\Lambda/N$ for the lattice Λ , can finally be written as:

$$f_\Lambda/k_B T = -p \log 2 - \frac{z}{2} \log(1+v^2) - \frac{1}{2} \int \frac{d^2 k}{(2\pi)^2} \log \det [\mathbf{1} - v \mathbf{W}_\Lambda(k_x, k_y)] . \quad (6)$$

The matrices $\mathbf{W}_\Lambda(k_x, k_y)$ are $m \times m$ matrices with $m = zp$. Here z is the coordination number of the lattice Λ , while p is the number of lattice sites in the unit cell of Λ . The values of m , z and p for the Archimedean lattices Λ are reported in Table 1.

4 Critical temperatures

At the phase transition the free energy becomes singular, from equation (6) we see that this can happen only if the argument of the logarithm becomes zero. For each Λ this can happen only for $k_x = k_y = 0$. To every lattice we associate the polynomials:

$$P_\Lambda(v) = \det (\mathbf{1} - v \mathbf{W}_\Lambda(0, 0)) . \quad (7)$$

The critical values of the high temperature parameter $0 < v_c < 1$ are the real solution of the equation

$$P_\Lambda(v) = 0 . \quad (8)$$

The polynomials $P_\Lambda(v)$ for the various Archimedean lattices are listed in Table 2. For all the lattices we considered, we found only one real solution of equation (8) in the interval $(0, 1)$. In all, but in the cases of the lattices $(3^4, 6)$ and $(3^2, 4, 3, 4)$, equation (8) has an

z	Λ	v_c	$k_B T_c/J$	$k_B T_c^*/J$
3	$(3, 12^2)$	$-\frac{1}{4} - \frac{\sqrt{3}}{4} + \frac{1}{2}\sqrt{3 + \frac{5\sqrt{3}}{2}}$	1.2315	5.0071
	$(4, 6, 12)$	$\sqrt{\frac{5+3\sqrt{3}-\sqrt{44+26\sqrt{3}}}{2}}$	1.3898	4.1363
	$(4, 8^2)$	$-1 - \frac{1}{\sqrt{2}} + \sqrt{\frac{5+4\sqrt{2}}{2}}$	1.4387	3.9310
	(6^3)	$\frac{1}{\sqrt{3}}$	1.5186	3.6410
4	$(3, 4, 6, 4)$	$\frac{1}{2} - \sqrt{\frac{\sqrt{3}}{2}} + \frac{\sqrt{3}}{2}$	2.1433	2.4055
	$(3, 6, 3, 6)$	$\frac{1}{2} - \sqrt{\frac{\sqrt{3}}{2}} + \frac{\sqrt{3}}{2}$	2.1433	2.4055
	(4^4)	$\sqrt{2} - 1$	2.2692	2.2692
5	$(3^4, 6)$	0.344296	2.7858	1.8757
	$(3^3, 4^2)$	$\frac{1}{3}$	2.8854	1.8205
	$(3^2, 4, 3, 4)$	0.32902	2.9263	1.7992
6	(3^6)	$2 - \sqrt{3}$	3.6410	1.5186

Table 3: For each Archimedean lattice, the exact critical value of the high temperature parameter v_c , of the Curie temperature T_c and of the dual Curie temperature T_c^* , are given. The Curie temperatures T_c and T_c^* are calculated from v_c using equations (9) and (10). The values for the lattices $(4, 6, 12)$, $(3, 4, 6, 4)$ and $(3^4, 6)$ were not yet known exactly and agree, within errors, with the numerical values of [22, 21]. The critical values for the lattices $(3^3, 4^2)$ and $(3^2, 4, 3, 4)$ agree with the exact results of [19]. Note that the lattices $(3, 4, 6, 4)$ and $(3, 6, 3, 6)$ have the same critical temperature.

explicit algebraic solution. The critical values v_c are listed in the column 3 of Table 3.

The critical temperatures T_c are related to the high temperature parameter v_c by the following relation:

$$T_c = \frac{J/k_B}{\operatorname{arctanh} v_c}. \quad (9)$$

The values we found are given in the column 4 of Table 3. The exact Curie temperatures for all the lattices, except for $(4, 6, 12)$, $(3, 4, 6, 4)$ and $(3^4, 6)$, were already known in the literature. In particular, they can be found in the following references: (4^4) in [2, 3, 4], (3^6) and (6^3) in [6], $(3, 12^2)$ in [8, 13], $(4, 8^2)$ in [9, 10, 13], $(3, 6, 3, 6)$ in [7, 13], $(3^3, 4^2)$ in [19] and $(3^2, 4, 3, 4)$ in [19, 12, 11].

We have compared our exact results for the lattices $(4, 6, 12)$, $(3, 4, 6, 4)$ and $(3^4, 6)$ with the numerical values available from Monte Carlo simulations [22, 21] and they agree within numerical errors. This is an independent confirmation of the correctness of our

analytical calculations for this new critical values.

The critical temperatures for the lattices $(3^2, 4, 3, 4)$ and $(3^3, 4^2)$ were calculated in [19] using the same combinatorial approach we are using, and agree with our findings. The fact that we used lattices where all edges are of unit length, contrary to [19] who used a different “embedding” of the lattices by constructing them from a square lattice adding diagonal links, shows that the critical temperatures depend only on the topology of the lattice and not on the particular representation of it. In fact, different embeddings of the same lattice lead to different random-walk matrices $\mathbf{W}_\Lambda(0, 0)$. This give rise to different polynomials $P_\Lambda(v)$, that instead have the same roots in the interval $(0, 1)$. The fact that the Curie temperatures depend only on the topology of the lattice is understood from the fact that the function $\Phi_\Lambda(v)$, which counts the number of closed even graphs, is a topological property of the lattice which is independent of the embedding.

Note that the lattices $(3, 4, 6, 4)$ and $(3, 6, 3, 6)$ have the same Curie temperature. This comes from the fact that the relative polynomials $P_{(3,4,6,4)}(v)$ and $P_{(3,6,3,6)}(v)$ have a common factor with root in the interval $(0, 1)$. This may suggest that the critical probabilities p_c for correlated percolation (also know as bootstrap percolation) on this lattices are equal.

Using the critical values for the high temperature parameter v_c found for the Archimedean lattices, we can calculate the Curie temperatures for the Laves lattices from the relation:

$$T_c^* = -\frac{2J/k_B}{\log v_c}, \quad (10)$$

which follows from duality, as shown in [2]. The values of the Curie temperatures for the dual lattices Λ^* are reported in collum 5 of Table 3.

5 Conclusions

We calculated the exact Curie temperatures for the two dimensional Ising model on all Archimedean and Laves lattices using the combinatorial approach of Feynman and Vodvicenko. This results are summarized in Table 3. In the particular case of the lattices $(4, 6, 12)$, $(3, 4, 6, 4)$, $(3^4, 6)$ and their duals $[4, 6, 12]$, $[3, 4, 6, 4]$, $[3^4, 6]$ our results were known in the literature only approximately from Monte Carlo simulations. This numerical results agree, within errors, with our analytical findings. The universal character of the phase transition is reflected in the singularity of the free energy, which is logarithmic ($\alpha = 0$) for all lattices. The Curie temperatures are not universal and we checked that they depend only on the topology of the lattice, but not on the particular embedding of it. The table of critical temperatures we compiled can be a useful reference to future

numerical and theoretical work on the Ising model on a large class of two dimensional lattices.

Acknowledgments

I would like to thank Prof. K. Binder for reading the manuscript and for useful discussion and suggestions.

References

- [1] R. Peierls, Proc. Camb. Philos. Soc. **32**, (1936) 477.
- [2] H.A. Kramers and G.H. Wannier, Phys. Rev. **60**, (1941) 252.
- [3] L. Onsager, Phys. Rev. **65** (1944) 117.
- [4] B. Kaufman, Phys. Rev. **76** (1949) 1232.
- [5] C.N. Yang, Phys. Rev. **85** (1952) 808.
- [6] G.H. Wannier, Phys. Rev. **79** (1950) 357.
- [7] K. Kano and S. Naya, Prog. Theor. Phys **10** 2 (1953) 158-172.
- [8] I. Syozi in *Phase Trasitions and Critical Phenomena*, C. Domb and M. S. Green eds. (1972) Wiley, New York, v. 1 pag. 269.
- [9] T. Utiyama Prog. Theor. Phys. **6** (1951) 907.
- [10] V. G. Vaks, A. I. Larkin and Yu. N. Ovchinnikov, *JETP* **22** 820 (1966).
- [11] Viktor Urumov, J. Phys. A: Math. Gen. **35** (2002) 7317-7321.
- [12] J. Strecka, Phy. Lett. A **349** (2006) 505-508.
- [13] V. Matveev and R. Shrock, J. Phys. A **28** (1995) 5235, arXiv: hep-lat/9412105.
- [14] M. Kac and J. C. Ward, Phys. Rev. **88** (1952) 1332.
- [15] R. P. Feynman, *Statistical Mechanics*, Benjamin/Cummings, Reading, MA, 1972.
- [16] N. V. Vdovichenko, *Sov. Phys. JETP* **20** (1965) 477-9.
- [17] S. Sherman, J. Math. Phys. **1** 202 (1960).

- [18] T. Morita, J. Phys. A: Math. Gen. **19** (1986) 1197-1205.
- [19] C.J. Thompson and M.J. Wardrop, J. Phys. A **7**, L65 (1974).
- [20] B. Grünbaum and G. Shepard, *Tilings and Patterns: an Introduction*, Freeman, 1989.
- [21] K. Malarz, M. Zaborek and B. Wrobel, TASK Quarterly **9** (2005) 475, arXiv: cond-mat/0506436.
- [22] F. W. S. Lima, J Mostowicz and K. Malarz, arXiv: 1001.3078 [cond-mat.stat-mech].
- [23] P. Fonseca and A. Zamolodchikov, J. Stat. Phys. **110** 527 (2003).
- [24] G. Mussardo, *Statistical Field Theory*, Oxford University Press, 2009.
- [25] M. Kardar, *Statistical Theory of Fields*, Cambridge University Press, 2007.